Glutaric acid, cyclohexylmethyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C25H30O5/c26-24(28-18-20-9-3-1-4-10-20)15-8-16-25(27)29-19-21-11-7-14-2

InchiKey: OHAMVGAAFQFREY-UHFFFAOYSA-N

Formula: C25H30O5

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 410.50

Physical Properties

Property code	Value	Unit	Source
gf	-173.58	kJ/mol	Joback Method
hf	-665.24	kJ/mol	Joback Method
hfus	46.80	kJ/mol	Joback Method
hvap	97.61	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.816		Crippen Method
mcvol	325.480	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	3254.00		NIST Webbook
rinpol	3254.00		NIST Webbook
tb	1024.29	K	Joback Method
tc	1264.61	K	Joback Method
tf	610.80	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.30	J/mol×K	1024.29	Joback Method
cpg	1109.03	J/mol×K	1064.34	Joback Method
cpg	1119.85	J/mol×K	1104.40	Joback Method
cpg	1128.80	J/mol×K	1144.45	Joback Method
cpg	1135.95	J/mol×K	1184.50	Joback Method
cpg	1141.35	J/mol×K	1224.55	Joback Method
cpg	1145.04	J/mol×K	1264.61	Joback Method
dvisc	0.0002337	Pa×s	610.80	Joback Method

dvisc	0.0001272	Pa×s	679.71	Joback Method
dvisc	0.0000775	Pa×s	748.63	Joback Method
dvisc	0.0000513	Pa×s	817.54	Joback Method
dvisc	0.0000362	Pa×s	886.46	Joback Method
dvisc	0.0000269	Pa×s	955.38	Joback Method
dvisc	0.0000208	Pa×s	1024.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392130&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume